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LASER-INDUCED FLAME KERNEL EVOLUTION WITH LES MODELING

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ABSTRACT

The present study investigates the comparison of numerically analyzed flame kernel evolution with experimental results from literature for the propane-air mixture at 0.12 MPa and 300K initial pressure-temperature conditions. The numerical analysis was done with ANSYS fluent software using RANS k- ε, k-ω SST, and LES turbulent models. The user-defined spark geometry was developed based on the Nd: YAG 1064 nm laser specifications. Results obtained predicted that the third lobe formation using the LES turbulent model was more promising than RANS models. The validated model was used to carry out analysis for equivalence ratios from 0.8 to 1.2. The kernel development started at 150 µs, 90 µs, and 135 µs for ϕ=0.8, 1, and 1.2 respectively. The flame kernel evolution was found prominent for stoichiometric conditions compared with lean and rich conditions.

KEYWORDS:Laser Ignition, LES Modelling, Flame Kernel Evolution & Flame Travel

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Original Article

INTRODUCTION

The combustion process should be initiated by a reliable ignition source to achieve the smoothness and stability of the process. The laser ignition is more superior to conventional spark-plug ignition, especially for initial flame kernel evolution speed [1]. Investigations on new ignition technologies have been carried out by many researchers from the last two decades, which includes the plasma jet ignition, rail plug ignition, laser ignition, flame jet ignition[2]. Laser-induced ignition is becoming one of the most promising ignition technology. Experimental studies on laser the ignition have been proved the potential advantages of laser-induced ignition over traditional electric spark ignition [3,4,5,6]. For example, laser ignition is an excellent point energy source which calculates precisely an exact amount of energy and its deposition rate. Engine misfiring and ignition delay period is possible to reduce using the facility of the flexibility of selecting laser ignition locations within the combustion chamber. Laser ignition has precise control on ignition timing; it also reduces the heat losses due to nonappearance of material in the vicinity of ignition location, increasing the lifetime of the laser ignition system. The electrical breakdown process initiated with energy transfer from the laser to plasma formation leads to shock waves generation and kernel formation followed by propagating flame [5,7]. Early-stage flame kernel development depends predominantly on the ignition source used for the initiation of combustion. In previous studies, significant research has been done on laser-induced combustion in engines as well as constant volume combustion chambers, whereas the research related numerical analysis of early-stage flame kernel development is still limited.

Bradley et al. carried out the fundamental studies on laser-induced combustion of the propane-air mixture. The detailed study of flame kernel formation has been carried out considering the gas dynamics. It was predicted that the gas dynamics effects of radiation waves at the plasma location are responsible for the change in shape and

size of kernel producing the third lobe. Flame initiation and growth in the early stage of methane-air laser-induced combustion carried out by Hassan Mohamed et al. [8], which revealed that the flame grows back towards the laser due to the plasma which absorbs more and more heat from the laser. A similar kind of third lobe formation of the kernel was found by S. Nakaya et al. using close duel point laser ignition. During a single point ignition, the third lobe was observed, whereas it was suppressed with duel point laser ignition [9]. Flame kernel characterization study for the compressed natural gas-air mixture was carried out in a constant volume chamber at 373K and 1MPa by D. Srivastava et al. The shape of kernel observed was cylindrical initially for a short time, then spherical changing into toroidal for an intermediate duration, and spherical for longer time duration. Many researchers found such a kind of frontal lobe in the direction of the incoming laser.

This is characteristic of laser-induced plasma ignition, which was observed by Bradley et al. Early-stage flame kernel development for hydrogen-enriched natural gas (HCNG) with laser ignition at various hydrogen volume fractions, and Prasad et al. studied equivalence ratios. It was concluded that higher hydrogen concentrations with lower air-fuel ratios led to reduced combustion duration. The flame front travel in the vertical axis was identical, but it was faster towards the laser direction compared to the opposite one [10].

The flame kernel becomes ellipsoid shape expanding fast in the horizontal direction giving rise to third lobe formation. The above literature gives significant knowledge about the experimentation carried out on various fuels using laser ignition, whereas B. Mewes et al. [11] developed the analytical laser ignition model to find the minimum laser pulse energy. Multiple models from open literature were connected and validated with the experimentation of hydrogen and methane fuel for the physical phenomenon of laser ignition, e.g., gas breakdown, laser light absorption coefficient, etc. Different parameters like adiabatic flame temperature, laminar flame speed, activation energy were estimated using CANTERA software. The comparative results achieved were highly accurate for model properties. It was observed that the ignition of methane was more complicated than the ignition of hydrogen. The results predicted from the model were found in good agreement with the measured one. Numerical analysis of the laser combustion of hydrogen-air was also investigated by [12]et al. In his work, the study of flame evolution in the homogeneous turbulent field of air was carried out. Seven species and eight reactions of hydrogen-air combustion were used in a finite rate reaction model. It was predicted that chemical reaction starts at the hot core zone, and the blast waves so formed keeps the un-burnt mixture separated from the hot core zone, which stops the further growth of its surface for some time. As the blast wave moves downstream, radial flow velocity decreases, and due to the high temperature of the hot core zone, the auto-ignition of the unburnt mixture takes place. This process was followed by the initiation of combustion. The authors also studied the numerical simulation of laser ignition using single and double laser pulses in quiescent air. [13]. The effect of successive two pulses on laser intensity, absorption rates, and shock wave propagation has been studied in detail. It was found that the amount of energy absorbed is higher, as the loss in shock wave radiation was less during the second pulse. Finally, in a recent study carried out by S. S. Shiva et al. investigated the laser-induced plasma generation and shock wave formations using a two-dimensional model for 50 to 150mJ laser ignition energies [14]. The plasma expansion was found to be unsymmetrical due to the higher pressure and temperature gradients along the laser axis than the radial axis. The elongation of plasma towards the laser was found more dominant. Similar kinds of plasma elongation results were observed by [15, 16], etc.

Amongst the published work on laser ignition, most of the work is on experimental research, whereas the research

related to the numerical analysis of flame kernel evolution indeed limited. In the present study, the numerical analysis of flame kernel evolution for a propane-air mixture using various turbulent models was investigated. A user-defined spark ignition model was developed to give the spark location, initial shape, and size. The results obtained from simulations were validated using the experimental results of Bradley et al. for the ϕ=1 at 0.1 MPa. Using the validated model, further simulations were carried out for lean and rich fuel conditions of equivalence ratio ranging from 0.8 to 1.2.

NUMERICAL PROCEDURE

Physical Domain

The physical domain used for simulation was a sphere, as given in the literature [5].

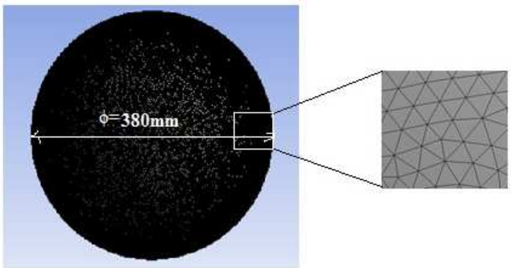


Figure 1: Model for Spherical Constant Volume Vessel [5].

The simulation was carried out for a time step size of 5 microseconds. Table1 gives the mesh statistics used for simulation

Table 1: Mesh Statistics

Property	Value
Number of Nodes	10009245
Mesh Type	Tetrahedral
Average Skewness	0.21
Orthogonal quality	0.9

Boundary Conditions and Simulation Models

The numerical simulation of laser ignited propane-air mixture was carried out using a spherical bomb of specification resemblance with published research on experimentation by Bradley et al. [5]. The simulation tool used for numerical analysis was commercial CFD software Ansys Fluent[18].

Table 2: Boundary Conditions for Simulation

Parameter	Value
Initial temperature	300K
Operating pressure	0.1MPa
Spark energy	23mJ
Spark duration	5.5ns
Laminar flame speed (m/s)	0.32, for ϕ=0.80.34, for ϕ=0.9, 0.38, for ϕ=10.37, for ϕ=1.1, 0.356, for ϕ=1.2[17]

To simulate the turbulent combustion flow, a Navier-Stokes equation with energy, continuity, and momentum was used along with the species conservation equation. The random and complex nature of turbulence is essential in the formation of flame evolution. The present work gives the comparative study of flame evolution using k-ε, k-ω, and LES turbulence model. The former two are RANS models, whereas the LES falls between RANS and DNS models. Large

eddies resolved directly and modeling of small eddies carried out with the use of the sub-grid model. Modeling of turbulent eddy viscosity determines the momentum transfer caused by turbulent eddies. Turbulent eddy viscosity was modeled by Smagorinsky Lily sub-grid scale. Radiation losses to the wall during turbulent combustion are essential in combustion application as it accounts for around 96% of total heat loss. The turbulence in combustion may have a substantial impact on radiation heat transfer; hence, to consider the turbulence and chemistry together, the coupled calculations are needed. The P model of radiation was used for simulation, which only finds zeroth and first-order moments of expansion radiation intensity. The radiative absorption coefficient was calculated by using the following co-relation,

$$\mathrm{k}'_{\mathrm{e,1}} = 0.1645 \times 10^{-34} \times \frac{\mathrm{n}_\mathrm{e}^2}{\mathrm{T}^{1/2}}\left[1 - \exp\left(\frac{-13500}{\mathrm{T}}\right)\right] \quad (1)$$

Where, $\mathrm{n_e}$ is electron number density and T is plasma temperature.

Laser Spark Model

The laser spark was assumed to be cylindrical. The results obtained by experimentation carried out by Awanish et al. was also revealed that the height of the kernel was equivalent to cylinder diameter [3]. Physical domain shape and size of the laser ignited spark was determined by using the following co-relation[3].

$$\mathrm{r} = \left(\frac{2\lambda}{\pi}\right) \times \left(\frac{\mathrm{f}}{\mathrm{d}}\right) \quad (2)$$

$$\text{And } \mathrm{l} = \left(\sqrt{\pi} - 1\right) \times \frac{\theta}{\mathrm{d}} \times \mathrm{f}^2 \quad (3)$$

Where the spark domain is assumed to be cylindrical in shape with length, and radius r, is the focal length, is the laser wavelength, is the laser beam diameter, is the laser beam divergence.

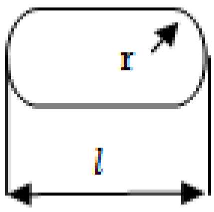


Figure 2: Physical Domain of Laser Spark.

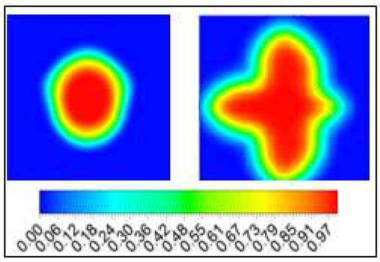


Figure 3: Comparison of Spark Developed with Spark Ignition and Laser Ignition/

The user-defined laser spark domain was generated, and the plasma temperature was given as 10000K [5]. Figure 3 shows the difference between the development of flame with spark ignition and laser ignition.

RESULTS AND DISCUSSIONS

Comparative Study Flame Kernel Evolution Using Different Turbulent Models

Flame Kernel Formation

Flame kernel evolution and flame propagation development take a time of several hundred microseconds. It was predicted from the experimental results of Bradley et al. that the gas dynamics and rarefaction waves play an important role in the formation of the third lobe [5]. The numerical results of flame kernel evolution using three turbulent models are shown in figure 2. Validation of numerical results was carried out by using the experimental results from the literature [5]. Figure 4

shows the images obtained by numerical simulation and experimental results from the literature[5] at various time instants. The rate of reaction progress with the k- ε model was comparatively shorter than the k-ω SST and LES model. The probable reason for this is the use of a single turbulent length scale to determine the eddy viscosity in the standard k- ε model, which is the dominant parameter for calculating the turbulent diffusion. Whereas in actual case, turbulent diffusion takes place due to all scales of fluctuation. Hence for complex phenomenon like combustion, where the variation in pressure gradients are severe, the k- ε model gives poor results. The k-ω SST turbulent model combines the near wall conditions and k- ε for away from wall conditions. This model has better numerical stability compared to k- ε model as, it uses dirichlet boundary conditions instead of damping functions. Compared with k- ε and k-ω SST turbulent models explained above, the shape and size of kernels obtained by numerical simulation using LES model, are in with good accordance with the experimental results from the literature. LES model resolves large eddies using filtered equations for modelling the less turbulence and calculating it for more time. This helps in reducing the errors originating from modelling of turbulence at small scale. Large eddies are equivalent to the characteristic length of fluid flow, and problem dependent because large eddies detection depends on geometry and boundary conditions. Dissipation of kinetic energy usually takes place due to the small eddies, which are filtered and modeled separately. The small eddies are more isotropic and comparatively less dependent on geometry. Hence LES attributed in better results.

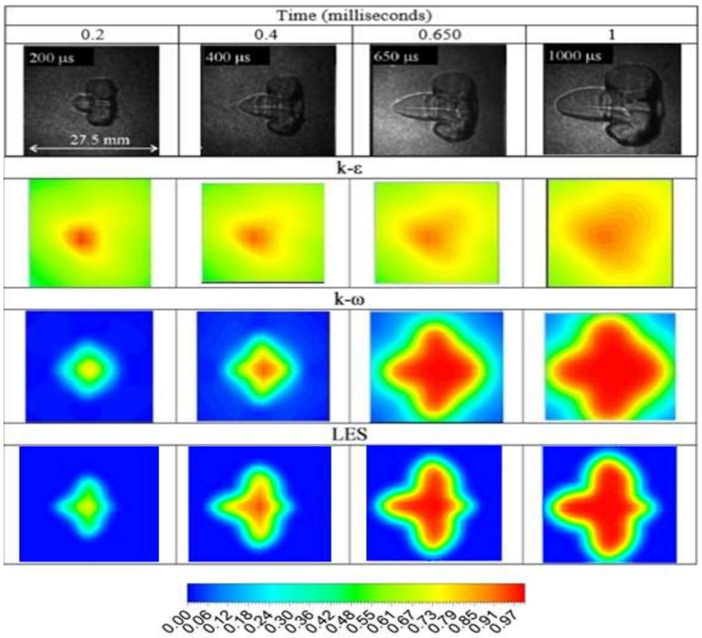
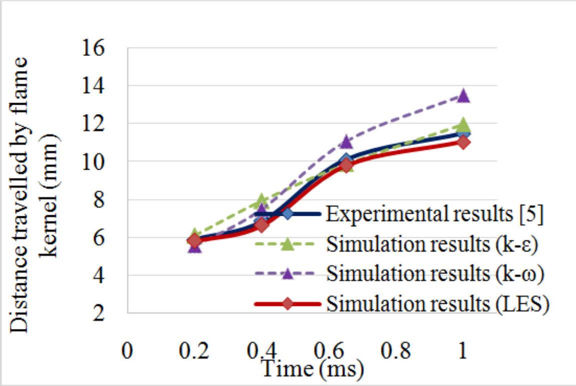


Figure 4: Flame Kernel Evolution Obtained with Numerical Simulation and Experimental Results from Literature for Propane-Air Mixture using different Simulation Models at phi=1, 0.1MPa and 363 K Initial Pressure-Temperature Conditions.

Flame Kernel Travel Towards Normal And Perpendicular Directions To Laser Source.

Figure 5 and (b) show the comparison between the experimental and numerical temporal displacement of the flame kernel in the directions normal and perpendicular to the third lobe using k- ε, k-ω and LES turbulent models.



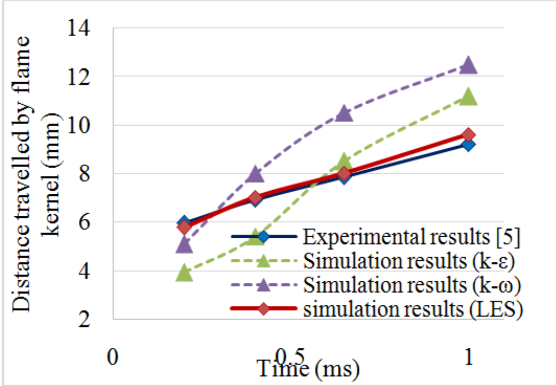


Figure 5:(a) Comparison in the Experimental and Numerical Temporal Variation of Flame Kernel Propagation Distance in Direction of the Third Lobe for a Breakdown of Propane-Air at 0.1 MPa, 300 K, for k- ε, k-ω SST and LES Model. (b) Comparison in the Experimental and Numerical Temporal Variation of Flame Kernel Propagation Distance in a Direction Perpendicular to the Third Lobe for a Breakdown of Propane-Air at 0.1 MPa, 300 K, for k- ε, k-ω SST and LES Model.

It was predicted that the simulation results obtained with LES turbulent model were in good agreement with experimental results. As discussed in the previous section, LES is more accurate as the large flow scales are resolved explicitly while small flow scales are modeled. The distance travelled using LES model and experimental results was found to be 9.54mm and 9.86mm at 0.65 milliseconds, respectively. The percentage error in the experimental and LES model found was 2.2% for normal to laser direction and 3.5% for perpendicular to laser direction, which was less than k- ε (error 15%) and k-ω (error 28%). Hence for flame travel in both directions, normal and perpendicular to the laser spark ignition source, the LES model simulation was found more accurate compared with the RANS turbulent models.

Flame Kernel Evolution of Propane-Air Mixture

The development of the third lobe is a significant parameter for combustion, as it helps in the mixing of plasma particles with surrounding particles. If this mixing takes place faster, then there were chances of shortening the lifetime of kernel, whereas if it is slower, then the kernel will remain smaller in size leading to late ignition or no ignition [5]. Flame kernel development as shown in Figure 6 predicted that the time required for flame evolution and third lobe was of several microseconds. The numerically obtained flame kernel images for the propane-air mixture shown in figure 5 are validated with the experimental results from the literature [5] for the equivalence ratio of ϕ=1. The validated model was further used to simulate an equivalence ratio of ϕ= 0.9, 1.1, and 1.2. It was observed that the reaction rate was higher for the chemically correct mixture. The volumetric growth of the flame kernel goes on increasing from ϕ=0.8 to ϕ=1 and then decreases as the mixture becomes rich. At ϕ= 0.8 the third lobe formed was weak compared with stoichiometric ratio due to the gas dynamics effect explained by [5].

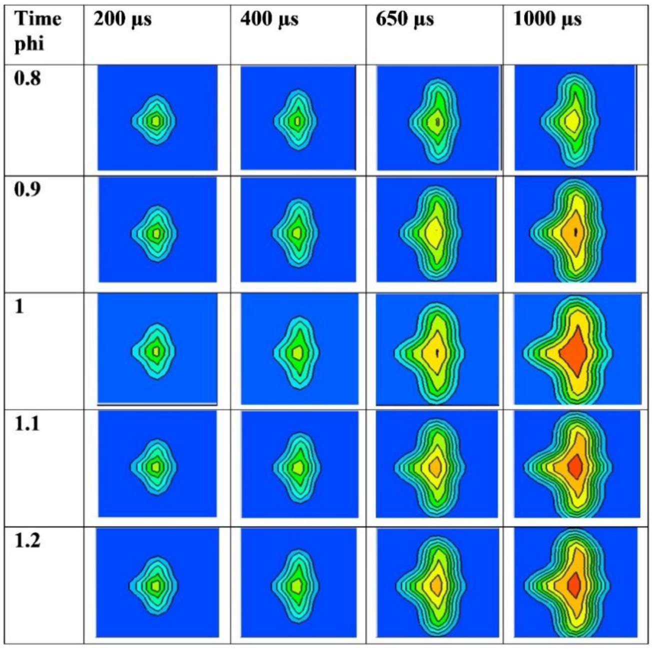


Figure 6: Flame Kernel Evolution of Propane-Air Mixture for an Equivalence Ratio of 0.8 to 1.2 at Different Time Steps at 0.1MPa and 363 K Initial Pressure-Temperature Conditions.

It was observed that the third lobe formation time instant was different for different equivalence ratios. For ϕ=1, the lobe formation started at 90 µs, which was earlier than for lean (ϕ=0.8) 150 µs and rich (ϕ-1.2)135 µs. This is because of the energy content and chemical compositions of the propane-air mixture at various equivalence ratios.

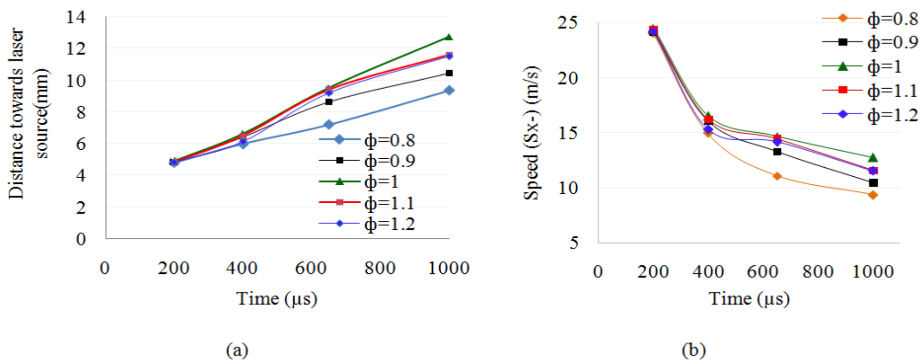


Figure 7: (a) Temporal Variation of Flame Kernel Propagation distance in the Direction of the Third Lobe (b) Speed, for a Breakdown of Propane-Air at Initial Temperature and Pressure condition of 300K, 0.1 MPa and Equivalence Range of ϕ=0.8 to ϕ-1.2 using LES Model.

Figure 7 shows the flame prorogation distance towards the laser source of propane-air mixture for various equivalence ratios. It was observed that the flame kernel propagation variation was almost linear for the selected range of equivalence ratio, which attributes in more or less constant flame velocity. For lean mixture at ϕ=0.8 flame propagation distance decreases with respect to time. The reason behind this may be the leaner mixtures are unable to continue the combustion in the third lobe after certain limits due to lower thermal energy contents, which further reduced flame velocity, as shown in figure 7 (b).

Similar kind of results was observed by A. Agarwal et al. [15]. However, at stoichiometric condition, i.e. when

ϕ=1, the flame travel distance towards the laser source was found to be higher compared with lean and rich conditions, as the laminar flame velocity at ϕ=1 is maximum.

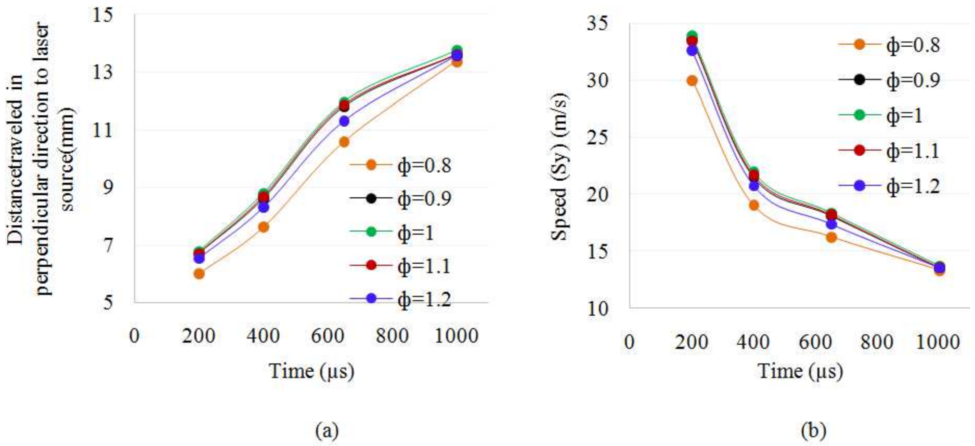


Figure 8: (a) Temporal Variation of Flame Kernel Propagation distance in a Direction Perpendicular (Y+ and Y-) to the Third Lobe (b) Speed, for a Breakdown of Propane-Air at Initial Temperature and Pressure Condition of 300K, 0.1 MPa and Equivalence Range of ϕ=0.8 to ϕ-1.2 using LES Model.

It was observed from the images obtained from the numerical simulation that the flame propagation travel in Y+ and Y- directions are identical, so only one direction flame propagation distance and speed reported here in Figure 8 (a) and (b). It was found that maximum flame kernel distance traveled was 13.75mm for ϕ=1, Flame propagation distance went on decreasing consistently for leaner mixtures and found lowest for ϕ=0.8. The results obtained by Awanish et al. also explained this phenomenon of increase of volumetric growth of the flame kernel with equivalence ratio. [17].

CONCLUSIONS

In this study, the laser-induced flame kernel evolution of propane-air mixture was investigated numerically and compared with the experimental results from the literature. The numerical simulation was carried out for three turbulent models, k- ε, k-ω SST, and LES model.

The temporal variation of the flame kernel evolution in normal and perpendicular to laser source directions inside the combustion chamber for different turbulent models were analyzed by interrogation of simulation images and compared with experimental results. The percentile error between experimental [5] and simulation results found was 8.205 and 9.38% for normal and perpendicular to laser source directions, which were in an acceptable range. The reason for error may be the experimental combustion chamber had optical access to the environment, which may lead to additional radiation heat loss effect, which is neglected in simulation. The RANS turbulence k- ε model also shows good accuracy with the literature, but the size of the kernel formed is distorted due time-averaging of fluctuation. The volumetric growth of stoichiometric mixtures was found increased compared with lean and rich mixtures. The third lobe formation was found evident using the validated model. The validated model will be used for future studies of different liquid fuels, using advancement in radiation models.

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